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MULTIPHYSICS NUMERICAL MODEL FOR THE ANALYIS OF CO_2 INJECTION IN CARBONATE ROCKS

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1 INTRODUCTION

In recent years, it was noticed an increased interest on the development of multi-physics constitutive models to provide reactive chemical analysis of the impacts of CO_2 injection in oil reservoirs. The movement was led by research groups interested in modelling Carbon Capture and Storage (CCS) and Enhanced Oil Recovery (EOR).

Given the rise in global temperature, it was detected that carbon dioxide plays an important role in global warming, contributing to more than 70% of gases of greenhouse effect, with residence time of over 100 years. According to Kyoto protocol, the signatory countries have defined commitments to limit greenhouse emissions. To accomplish the carbon reduction targets, it was created the Clean Development Mechanism (CDM), where developed countries could invest in projects to reduce greenhouse emission in developing countries, being these reductions accounted for carbon credits.

Aiming to fulfil target reductions on carbon emissions, interest grew on the development of solutions for carbon sequestration from the atmosphere. One of the most promisor long-term solutions is the injection of carbon dioxide in underground rocks or carbonate oil reservoirs. The injection of CO_2 in carbonates promotes acidification of underground water making it more prone to react and dissolve the rock porous matrix. With dissolution, the pore structure of the rock changes, modifying the permeability and hydraulic conductivity of the medium.

In order to quantify the long-term impacts of carbon capture by CO_2 injection in reservoirs, it is necessary to understand and quantify the chemical effects of dissolution in porous media, its impacts on rock structure and consequent change in underground flow [1]. In addition, it is necessary to account for the transport of chemical species and its contribution to the reaction. Continuous models were proposed taking into consideration the effect of reaction kinetics [2], diffusive effects [3], and both effects in two scales [4]. The two-scale model proposed by

Panga is similar to the model of heterogeneous catalytic reactors, but considers flow coupling, reaction/dissolution rates, and effects of mass transfer at pore scale. Indeed, the majority of the works on reactive modelling considers the diffusive-convective transport with source/sink term to represent chemical reaction with hydraulic coupling [5].

This work presents a straightforward implementation of a numerical model capable of evaluating the impacts of CO_2 transport in porous media, assessing dissolution and change in porosity in the rock matrix using the FEM.

2 MATERIAL AND METHODS

Chemical interaction between minerals and water originate from the chemical unbalance that persists in the system. Dissolution occurs when fluids are not saturated in respect to some minerals, making the product of ionic activity inferior to the equilibrium constant. In CO_2 injection processes, changes in chemical conditions occur locally given the dissolution of gas in the fluid within the reservoir. Considering the temperature and pressure of the fluid, the increase in CO_2 partial pressure favors the dissolution of carbonate minerals [6].

The porosity change can be computed through the volumetric quantity of minerals dissolved, which corresponds to an approximation to the mass balance. The macro description of dissolution patterns is very complex, being influenced by several factors, such as sample heterogeneity, reaction kinetics, and mass transfer [7].

$$\frac{\partial(\emptyset C_i)}{\partial t} + \nabla.(\boldsymbol{U}C_i) = \nabla.(\emptyset \boldsymbol{D_e}.\nabla C_i) - \ \vartheta_m R_m \ + \Gamma_i \tag{1}$$

A major number of experimental and theoretical studies analyzed the influence of dissolution processes on the physical chemical properties of porous media [8,9]. Mechanisms such as pore coalescence and flow channel formation involve complex effects [10].

To model reactive chemistry, we chose a continuous model approach, describing the phenomena in Darcy scale and an adaptation of the kinetic model from Chou [10], incorporating a term to describe the change on the porous superficial area, as proposed by Noiriel et al. The Finite Element method was chosen for domain discretization and to compute the transport equations and chemical reactions. To evaluate the change in porosity and permeability, the formulation proposed by Hao was implemented [11].

$$R_m = S_0 \left(\frac{\phi_t(1-\phi_t)}{\phi_0(1-\phi_0)}\right)^{\frac{2}{3}} k x_{CO_2} \tag{2}$$

Mineral reaction rate reads Eq. 2. and porosity change is derived directly from the reaction rate of calcite dissolution, as indicated in Eq. 3

$$\frac{\partial \phi}{\partial t} = -\vartheta_m R_m V_m \tag{3}$$

The proposed constitutive model of CO_2 injection in carbonates was implemented in the commercial software COMSOL Multiphysics ("COMSOL") and solved in a fully coupled scheme.

2.1 Coupling strategy

The dissolution of calcite, Eq. 4, solved in COMSOL considers the coupling of three physics: chemical reactions, transport of species and Darcy flow.

$$CaCO_3(s) + CO_2(g) + H_2O \leftrightarrow Ca^{2+}(aq) + 2HCO_3^-(aq) \tag{4}$$

The three physics are linked as described below:

- The transport of dissolved CO_2 in water is computed with transport of species physics. The input velocity field read in the convective term of the convection-diffusion equation Eq. 1 arises from the computed Darcy model;
- Updated species concentration arising from the dissolution reaction are computed in Chemical reaction module taking into consideration the reaction kinetics of the dissolution equation;
- The change in porosity is updated in Darcy model considering the reaction rate of calcite, Eq. 3.

2.2 Solution Method

The problem was solved with the non-linear Newton method, and solver MUMPS considering 723 degrees of freedom and simulation time of 15 hours, time step size 0.5s, solution time 6 min.

3 RESULTS

The proposed constitutive model of CO2 injection in reservoirs implemented in COMSOL was capable of following closely experimental data of carbonate rock dissolution described in the literature [12].

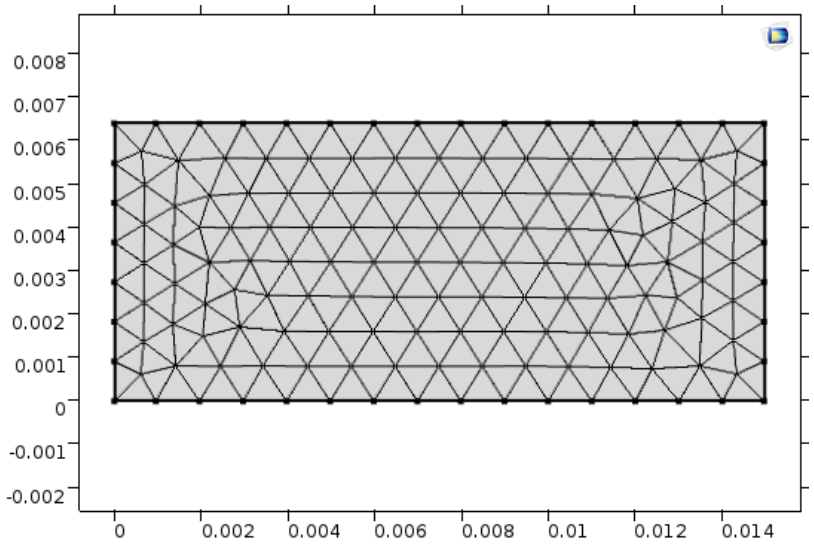

Figure 1: Mesh generated with linear triangular elements

Results from the numerical simulation lead to the identification of uniform porosity change in the porous media, as presented in figure 3.

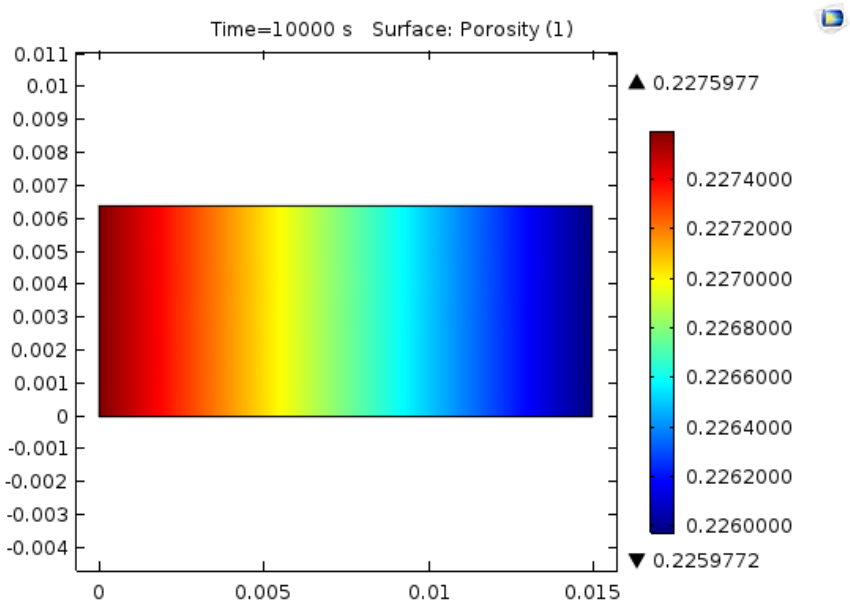

Figure 2: Porosity profile, recovering uniform dissolution, at 10,000s

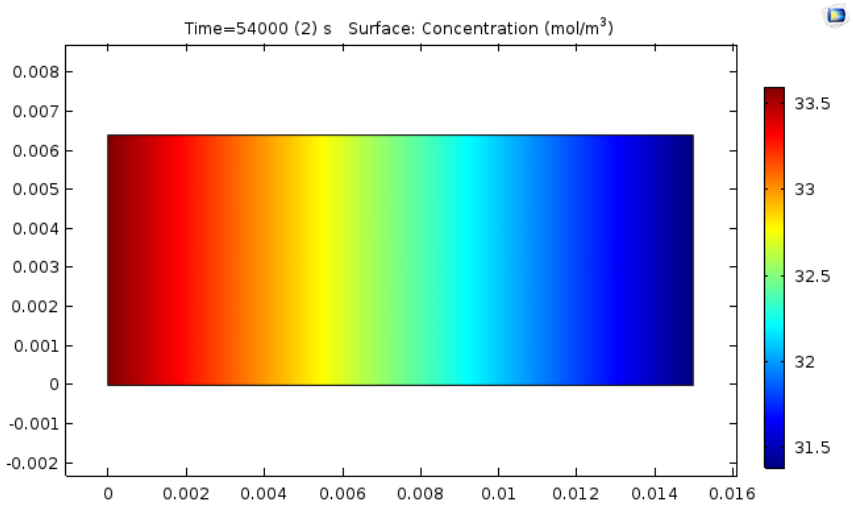

Figure 3: Transient results of CO2 concentration in COMSOL, at 54,000 s

In figure 4 the results from the numerical simulation in COMSOL were compared to experimental data from Noiriel [12](table 1).

Table 1: Noiriel Experimental data

Time (h)	Porosity (%)
0	20.3
9	24.7
15	30.2

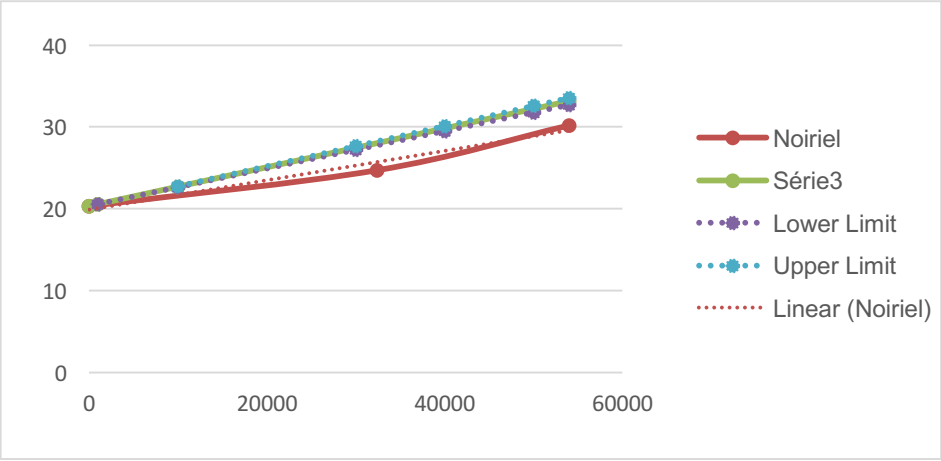

Figure 4: Transient results of porosity change in COMSOL and Noiriel data [12], porosity (%) vs. time (s)

4 CONCLUSIONS

- The continuous model for dissolution was able to recover the porosity changes when compared to the test reactive flow in real rock given initial data on rock porosity obtained with micrography of X-Ray.
- The straightforward approach used for modeling acidification in carbonates is a good alternative for the study and optimization of projects related to CO2 injection in reservoirs in projects of EOR or CCS.
- The fully coupled strategy has significant computational cost; alternative coupling strategies should be tested for larger scales and different dissolution patterns.

The simplified model presented in this paper does not account for precipitation of minerals, and may be extended accordingly [13].

5 ANNEX

Table 2: Variables

C_i	Concentration of species i
$\boldsymbol{D_e}$	Effective diffusivity
ϑ_m	Stoichiometric coefficient
R_m	Mineral reaction rate
$\boldsymbol{U}$	Velocity
Γ_i	Source / Sink term
S_0	Initial superficial area
x_{CO_2}	Molar fraction of CO2
V_m	Molar volume of calcite
k	Chemical kinetic constant
$\emptyset$	Porosity
ϕ_0	Initial porosity
ϕ_t	Current porosity

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